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Extreme thermodynamic conditions: novel stoichiometries, violations of textbook chemistry, and intriguing possibilities for the synthesis of new materials.

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Extreme thermodynamic conditions: novel stoichiometries, violations of textbook chemistry, and intriguing possibilities for the synthesis of new materials.

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As evidenced by numerous experimental and theoretical studies, application of high pressure can dramatically modify the atomic arrangement and electronic structures of both elements and compounds. However, the great majority of research has been focused on the effect of pressure on compounds with constant stoichiometries (typically those stable under ambient conditions). Recent theoretical predictions, using advanced search algorithms, suggest that composition is another important variable in the search for stable compounds, i.e. that the more stable stoichiometry at elevated pressures is not *a priory* the same as that at ambient pressure. Indeed, thermodynamically stable compounds with novel compositions were theoretically predicted and experimentally verified even in relatively simple chemical systems including: Na-Cl, C-N, Li-H, Na-H, Cs-N, H-N, Na-He, Xe-Fe. These materials are stable due to the formation of novel chemical bonds that are absent, or even forbidden, at ambient conditions.

Tuning the composition of the system thus represents another important, but poorly explored approach to the synthesis of novel materials. By varying the stoichiometry one can design novel materials with enhanced properties (e.g. high energy density, hardness, superconductivity etc.), that are metastable at ambient conditions and synthesized at thermodynamic conditions less extreme than that those required for known stoichiometries. Moreover, current outstanding questions, “anomalies” and “paradoxes” in geo- and planetary science (e.g. the Xenon paradox) could be addressed based on the stability of surprising, stoichiometries that challenge our traditional “textbook” picture. In this talk, I will briefly present recent results and highlight the need of close synergy between experimental and theoretical efforts to understand the challenging and complex field of variable stoichiometry under pressure. Finally, possible new routes for the synthesis of novel materials will be discussed.

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